Quality Assurance Project Plan for

Surface Water Transport of Hydraulic Fracturing-Derived Waste Water

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QA Category: 1

HF Project #5a

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/s/ 2/22/12

James W. Weaver, Principal Investigator — Date

APPROVALS:

/s/ 2/22/12

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/s/ 2/22/12

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A2 Contents

A3 Distribution List

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Contract project participants:

Victor Murray, Shaw Environmental

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Student Services Contractor to be determined

A4 Project Organization

Stephen Kraemer, Research Hydrologist, National Exposure Research Laboratory (NERL), Ecosystems Research Division (ERD), Regulatory Support Branch (RSB), Athens, GA, and ***Modeling Technical Research Lead***, ORD Hydraulic Fracturing study. Responsibilities: Review and approval of QAPP, project coordination, and review of draft deliverables .

Steve Vandegrift, Quality Assurance Manager NRMRL, GWERD, Ada, OK. Responsibilities: QA review and approval of QAPP and final report, QA guidance, and management of QA audits.

Jim Weaver, Research Hydrologist, NRMRL, GWERD, SRB, Ada, OK. Responsibilities: task oversight, scenario development, modeling, code development, literature review, QAPP preparation and implementation.

Susan Mravik, Soil Scientist, NRMRL, GWERD, SRB, Ada, OK. Responsibilities: Scenario development, data collection, model application, contractor oversight.

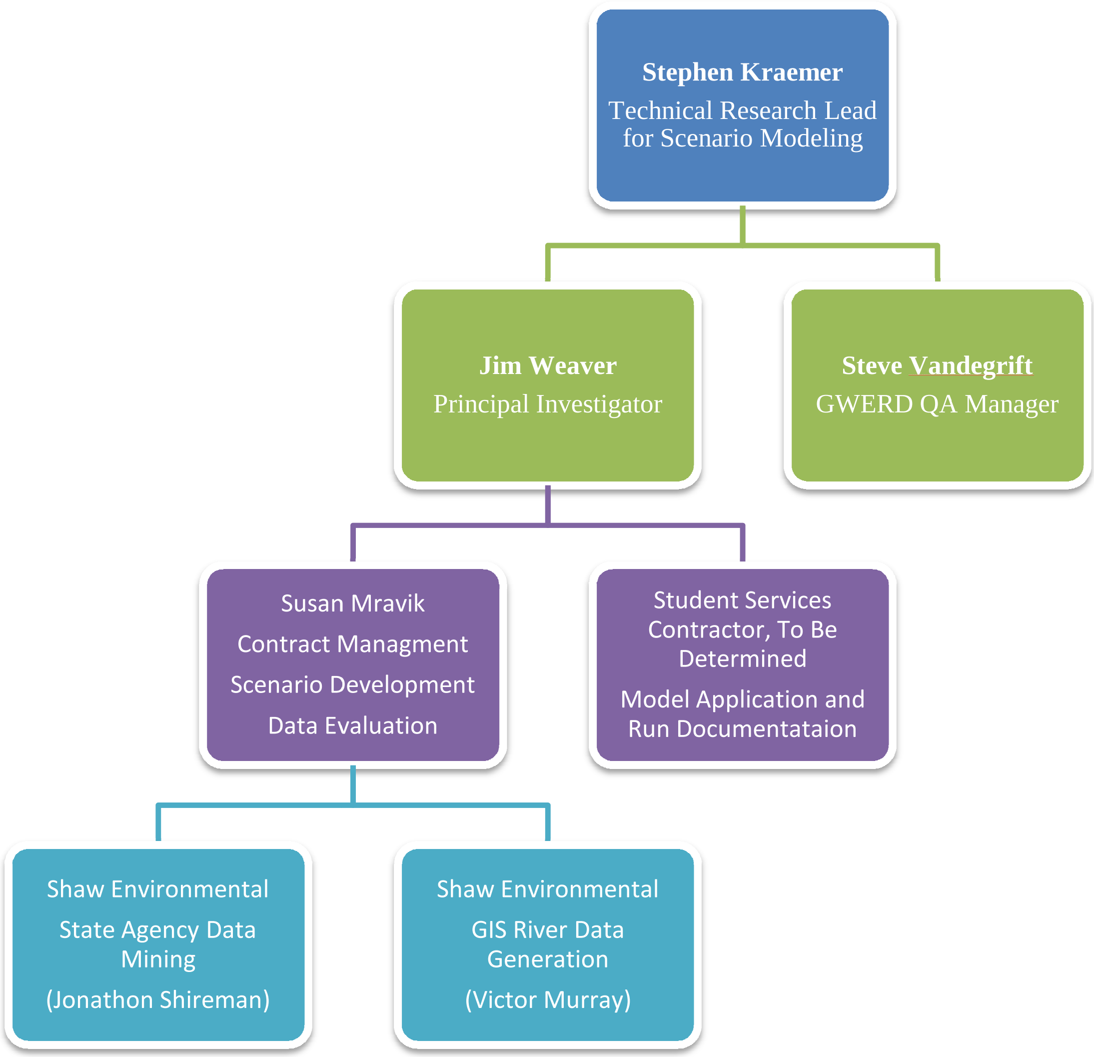
Contract project participants, TBD

Victor Murray, Shaw Environmental, Map preparation, river parameter determination,

Jonathon Shireman, Shaw Environmental, data mining from state agencies

Student Services Contractor, to be determined in FY2012

Organization Chart



A5 Problem Definition and Background

Disposal of hydraulic fracturing (HF) flow-back and production water to treatment plants and subsequent release to surface waters presents potential drinking water contamination problems. These might result from release of naturally occurring radioactive materials (NORMs), elevated concentrations of chloride and bromide, which lead to disinfection byproduct formation in water treatment plants, and possibly other compounds that are present in treated waste waters. NORMs have been characterized as simply gross alpha decay or by identification of specific nuclides, including radium and uranium 235. Increased chloride and bromide present potential problems as they increase the formation of both regulated and unregulated disinfection byproducts. Bromide, particularly, could be a problem when chlor-amination is used for treatment and can lead to a family of unregulated disinfection byproducts. If sufficient in magnitude, HF wastes might expand this problem to areas with low naturally occurring bromine

Transport in rivers from discharges to drinking water intakes is potentially influenced by a number of processes that include river discharge, longitudinal and transverse mixing, turbulent diffusion, volatilization, sorption and decay. River discharge varies from point-to-point and day-to-day as it responds to changing rainfall and runoff. Waste is discharged to rivers at various locations, rates and compositions. Publically owned treatment works (POTWs) and industrial treatment plants may accept HF wastes on an intermittent basis and the composition, volume and frequency of discharge from these is expected to be variable. There may be blending of HF waste with other waste water to reduce impacts to receiving waters.

HF flowback and production water disposal methods vary around the U.S. In some locations deep well injection is used, while others, notably Pennsylvania, allow treatment of wastes at waste water treatment plants. Recycling of HF flow-back and production water for use in additional HF operations decidedly plays a role in the quantity and quality of waste water. These issues have been widely publicized so that future changes in disposal practices are likely. In so far as possible, this project will be designed to provide the most usable results.

Objectives

The primary objective of this project is use models to illustrate the conditions under which disposal of hydraulic fracturing wastes might cause negative impacts on drinking water resources.

This objective will be met through two sub-objectives

1) Simulating a generic river situation using the most accurate descriptors as possible to provide a first order view of problematic conditions.
2) Simulating one or more actual river networks to show potentially problematic conditions where exist given the actual locations of water intakes.

The project QAPP will be updated after the first set of results (the generic river simulation) is produced. This will allow for "lessons learned" to be incorporated into the QAPP for the watershed simulations. Since the modeling approach may be changed for the watershed-specific simulations, different tests will be undertaken for model sensitivity and uncertainty.

A6 Project/Task Description

Scenarios are to be developed to address surface water disposal of treated HF wastes. Definition of the scenarios provides the conceptual model for evaluation. The conceptual model includes definition of the river system, location of discharges and drinking water intakes, flow rates, discharge rate and composition, transport and transformation processes, required dimensions, and others. Since one focus should be on long-term impacts, the analysis could start with a baseline analysis. This baseline could be defined as both a steady flow in the river network and a steady discharge of treated HF waste, which represent a specific type of release into representatively-flowing river. Deviations from this baseline can address impacts at low flow or drought conditions where discharge might decrease and water demand might increase and conversely a high flow conditions. Waste disposal involving varying volumes or numbers of discharges (both increase and decrease), time-dependent loadings of discharges and varying concentration of effluents are a second set of factors influencing the scenarios. These two sets of factors generate a series of potential impacts for consideration of impacts at drinking water intakes.

Data requirements

The Monongahela, Allegheny, and Susquehanna River networks have been used for disposal of treated HF waste waters. These are likely candidates for scenario analysis. Data associated with these rivers that are needed for this study include the geometry of the river network, data on flows and bathymetry, where available from the U.S.G.S. river monitoring network. USGS tracer studies performed on these rivers (e.g., studies on the Susquehanna) may be useful for estimating travel time and effective diffusion coefficients. Data on the quantity and quality of HF discharges are needed. Sources include EPA, DOE and State Agency reports. Existing discharge/drinking water intake data will be sought to test the modeling approach for specific situations.

Model selection

The characteristics of the chosen scenarios, data and availability of model codes will be used to select the appropriate code or codes for simulation. Some simple transport calculations or analytical solutions to the transport equation may be useful in a rough screening analysis. Beyond these some of the major transport codes will be evaluated for their match to the scenario characteristics: Water Analysis Simulation Package (WASP) developed by EPA, QUAL2K distributed by EPA, RMA4 developed by the Army Corps of Engineers, and others are under consideration, but the choice of code will follow the dictates of the scenario conceptual model. Within the definition of the conceptual model, uncertainty analyses will be undertaken to assess potential uncertainties.

As an alternative the empirical/statistical approaches pioneered by Holley and Jirka (1986) and Jobson (1996) will be evaluated for use in the generic river simulation phase of the project. These models are based on compilations of tracer data. The advantage of these approaches for generic screening is that they 1) are based on rivers from around the U.S., 2) use tracer data from actual experiments, so that they do not require assumptions on travel times and dispersion coefficients and 3) are complimentary to the simulation programs described above.

Jobson's technique was developed for application to instantaneous releases in single reaches, which are characterized by single values of slope, discharge, average annual discharge, and drainage area. Thus the method will be generalized for 1) rivers with varying reach properties, 2) branching river networks, 3) continuous injections of specified duration. The code will be implemented in Java and tested against available tracer data. Comparisons will be made and documented to one or more of the models mentioned above.

Tracer-based Empirical Transport Estimation

Jobson (1996) developed an empirically-based approach to estimate travel time and longitudinal dispersion in rivers and streams. The method relies on compiled tracer data so that the result is largely based on observation of transport in real systems. The motivation for this approach is stated by Jobson

> "In general there are no reliable methods of prediction dispersion coefficients (mixing rates) from commonly available hydraulic information. Stream velocities, typically predicted by use of a flow model, generally require very detailed channel geometry and flow resistance coefficients, which are seldom available. The availability of reliable input information is, therefore, almost

always the weakest link in the chain of events needed to predict the rate of movement, dilution, and mixing of pollutants in rivers and streams."

Much of this statement remains true fifteen years later, although advances have been made in predicting longitudinal dispersion coefficients (see below). The data-limitation problem can be overcome by using tracer data, as noted by Jobson:

> "Measured tracer-response curves produced form the injection of a known quantity of soluble tracer provides an efficient method of obtaining the data necessary to calibrate and verity pollutant transport models."

Jobson's (1986) procedure relies on a series of regression formulas he developed from tracer data. They represent, collectively, the response of rivers and streams to solute injection experiments. In order to compare data from rivers of diverse sizes and injections of various amounts, the data are normalized by the mass of injection, flow rate, and mass lost to sorption or degradation. The remaining variable, the longitudinal dispersion, is assumed to be comparable given this normalization (Jobson, 1996). Jobson (1996) then used data from 60 rivers, 109 tracer injections, and 422 cross sections to develop the regression equations. The river discharges ranged from a mean annual discharge of 1.3 m^3/s in a small creek to 11,000 1.3 m^3/s in the Mississippi River. The slopes ranged from 36.0 m/km in the creek to 0.01 m/km in the Mississippi River.

From the 422 cross sections that had data on annual mean flow, Jobson found that the unit peak concentration was represented by

$$C_{up} \;=\; 1025\, T_p^{-0.887}$$

where C_{up} is the peak unit-concentration [sec^{-1}] and T_p is the time to peak concentration in hours. A unit concentration, C_u [T^{-1}] , is determined from

$$C_u \;= 1\, x\, 10^6\, \frac{C}{R_r} \frac{Q}{M_i}$$

where C is the concentration [M/L^3], R_r is the recovery ratio [dimensionless], Q is the stream discharge [L^3/T], and M_i is the mass injected [M]. The recovery ratio is defined as the mass passing a cross section to the mass injected. Although called a concentration, the unit concentration is actually partially non-dimensional mass flux (mass flux per unit mass of injected solute), which retains the time unit in the denominator. The factor of 1×10^6 is a convenience. Jobson refined the estimate of peak unit-concentration, by including the ratio of river discharge, Q [L^3/T] to mean annual river discharge Q_a [L^3/T]. The resulting equation is

$$C_{up} \;=\; 857\, T_p^{-0.760\left(\frac{Q}{Q_a}\right)^{-0.079}}$$

In several cases, data for a river show dependence on the relative discharge (Q/Q_a), although this is not always the case (Jobson, 1996, figures 4 through 7).

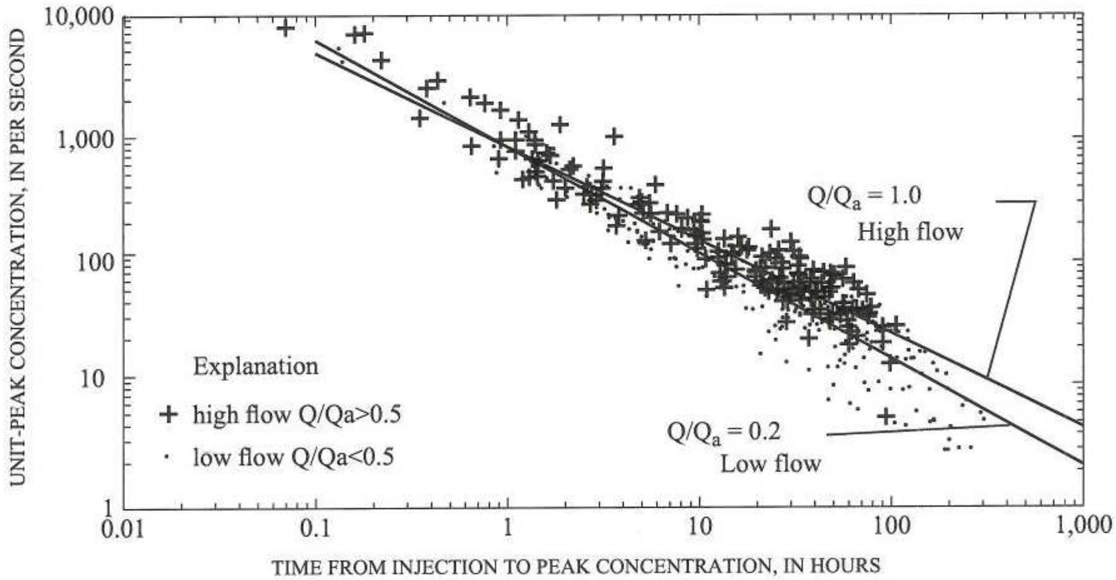


Figure 1 unit-peak concentration regression formulas developed by Jobson (1996).

Variables that influence the transport time include the drainage area, D, [L^2], the reach's slope, S, [dimensionless], the mean annual discharge, Q_a, [L^3/T], and the discharge at time of measurement, Q, [L^3/T]. These were used in forming regression formulas for travel time of the peak concentration. The most accurate equation for the peak velocity, V_p, [m/s] contained all variables:

$$V_p \qquad 0.094 + 0.0143\, D'^{0.919} \quad {}'^{-0.469}_{a}\, S^{0.159} \, \frac{}{D}$$

where D' is the dimensionless drainage area defined b $D' \quad D^{0.125}\sqrt{g}\big/_{a}$, g is the acceleration of gravity [L/T^2], and Q' is the dimensionless discharge defined by Q/Q_a. Discharge Q is expressed in m^3/s, and drainage, D, in m^2 for this and the following regression equations. Alternate regressions were developed for situations where some of these variables are unavailable. When slope is not available,

$$V_p \qquad 0.020 + 0.051\, D'^{0.821} \quad {}'^{-0.465}_{a} \, \frac{}{D}$$

When slope and mean annual discharge is unavailable,

$$V_p \qquad 0.152 \; + \; 8.1\, D''^{0.595} \; \frac{}{D}$$

where the dimensionless drainage area was redefined by $D'' \qquad D^{0.125}\sqrt{g}\big/$.

Bounding estimates that give velocity values greater than 99 percent of the data points, $V_{p_{max}}$, were given for each of these situations:

$$V_{p_{max}} \qquad 0.25 + \; 0.02\, D'^{0.919} \quad {}'^{-0.469}_{a}\, S^{0.159} \; \frac{}{D}$$

$$V_{p_{max}} \qquad 0.2 \; + \; 0.093\, D'^{0.821} \quad {}'^{-0.465}_{a} \; \frac{}{D}$$

$$V_{p_{max}} \qquad 0.2 \; + \; 40.0\, D''^{0.595} \; \frac{}{D}$$

The time for the leading edge of the concentration distribution, T_l [hours], was found to be highly correlated to the peak arrival time, following

$$T_l \qquad 0.890\, T_p$$

The time for the trailing edge of the concentration distribution, T_{d10} [hours], was estimated from

$$T_{d10} \qquad 2 \quad 10^6 \big/ C \;\; _p$$

an equation which is based on the assumption that the area under the unit concentration curve is 1×10^6, and that half of the mass lies between the peak concentration and a point where the concentration is one tenth the peak value.

Because limited data from Pennsylvania streams and rivers were included in Jobson's formulas, Reed and Stuckey (2002) evaluated the Jobson equations for use in the Susquehanna, Delaware, and Lehigh River basins. They found that the equations show good agreement with time-of-travel studies at low and moderate flow rates. At high flow rates, the Jobson equations over-predicted travel times, and so, Reed and Stuckey (2002) developed a modified equation. Reed and Stuckey (2002) recommend using the Jobson equation for low to moderate flow rates , where $Q/D^{0.73}$ is less than about 2. For higher values of $Q/D^{0.73}$, the modified equation that should be used is

$$\dot{V} \qquad 0.6067\, e^{\left[log_{10}\left(\dot{Q}/_{\dot{D}^{0.73}}\right)\right]}$$

where the velocity, $\dot{V}$, is expressed in ft/s, the discharge, ˙, in ft^3/s and the drainage area, $\dot{D}$, in $miles^2$.

<u>Definition and Testing of a Simplified Scenario (Objective 1).</u> A simplified generic scenario will be developed to assess the general characteristics of releases of treated water to surface waters. The conceptual model will consist of an idealized river section with generalized inputs and receptors. The inputs, however, will be generated from as realistic information as possible, given the constraints of time, required high-level quality assurance and data availability. The scenarios will be developed based on locations where discharges actually occur. Data on oil and gas waste disposal in Pennsylvania will be mined to generate these locations. These selections, in turn, determine the size and properties (slope, drainage area, annual discharge) of the river network. For example, Williamsport Pennsylvania was the location of HF waste discharges during the first half of 2011 (https://www.paoilandgasreporting.state.pa.us/publicreports/Modules/Welcome/Welcome.aspx). Williamsport is located on the West Branch of the Susquehanna River where data from USGS station 01551500 are available.

From this type of input the model is expected to be able to generate a general guide to releases of treated HF wastes that allows exploration of the ranges of parameters which generate or mitigate drinking water exposure. To make the simulation results realistic, actual locations will be used in the generic simulations, which presents a departure from the original plan for the project. The reason for this change is that 1) specific locations are needed to drive the Jobson (1996) empirical modeling approach, and 2) estimates of treated wastewater discharges are highly localized. By looking at specific locations where HF wastes are/were disposed, the results will be most defensible, because some drainage-ways in areas of intensive HF activity are not used for treated wastewater disposal.

<u>Selection of Test Watershed and Definition of Scenarios (Objective 2).</u>

The watersheds will be prioritized by the amount of available data. The most data-rich watershed will be selected first for development of a simulation and establishment of scenarios. The scenarios will include varying of the variables described above to develop watershed-specific versions of the simplified scenario described above, but with constraints built in from the location and nature of specific facilities. The results of the watershed scenarios will be compared against the generic simulations to determine the ability of the generic constraints to capture the watershed characteristics.

I. funding

Principle Investigator	**FY11**	**FY12**	**FY13**
Jim Weaver	FTE	FTE	FTE
Susan Mravik		FTE	FTE
Contract support		$50K	$50K
Contract support (SSA Student)		$50K	$50K

II. expected products (outputs) and impact (outcomes)

output: Report/paper on scenario modeling, report on analysis of waste disposal data, contributions to the 2012 report to congress, others to be developed

outcome: Assessment of conditions that make surface water discharge of treated HF waste problematic.

III. milestones and status

Aug 1, 2011: Completed and approved QAPP.

Oct 1, 2011: Draft summary of literature on surface water transport (intended as background material for 2012 report to Congress)

Dec 1, 2011: Transport model and associated analytical solutions selected; Generic scenario model described in draft document

March 1, 2012: Simulations completed for generic scenario; First draft of generic scenario results

March 31, 2012: Completed draft report of generic scenario results (provided as potential material for 2012 report to Congress); First watershed selected based on available data

July 1, 2012: Data compiled for watershed simulation, simulations begin

Dec 1, 2012: Draft report on first watershed simulation.

Jan 1, 2013: Further milestones to be developed, QAPP to be revised for the watershed application.

A7 Quality Objectives and Criteria

In this project the quality objectives are:

- To obtain data to support modeling studies that are of known quality
- To document the correct application of data interpretation and analysis methods.
- To document steps in model code development
- To perform simulation results where the trail from input data to model outputs is as transparent as possible.
- To assess uncertainty in the model results
- To retain records that document the activities of the project

Data with Known Quality

Data form the basis of inputs for the scenario modeling. These will be drawn from published peer-reviewed journal papers, federal agency reports, and state agency-accepted data. Information in these documents will be used to judge the quality of the data. Where available "supplemental information" from the papers will be used and saved as part of the quality documentation. See Section B9 for more detail.

Data Analysis Methods

Where necessary to interpret or manipulate data from various sources, the methods used will be documented in the lab notebook. Documentation will include the methods and their sources, example results with correctness verification and location of any spreadsheets or other resources used in calculation. The empirical methods developed by Holley and Jirka, 1986, and Jobson, 1995 are examples of where these approaches are likely to be used.

Documenting Code Development

Development of any code to implement a model shall be documented in laboratory notebooks of the project participants. A Java language code is anticipated to implement varying reach properties, tree-searching, uncertainty analysis, and multiple inputs for the Jobson (1996) empirical method. The code itself shall contain internal documentation to describe the functioning of the model. Model outputs and inputs shall be stored electronically according to the structure described in section A9. Test problems shall be referenced in laboratory notebooks (locations of electronic files) and described along with relevant results.

Simulation Results

The basis of simulation results will be documented by drawing a path from the input data to specific model results. This will be largely documented in the laboratory notebooks of the participants. The lab notebooks will be unique to this project. The documentation will include the development of a conceptual model for the transport scenarios, documentation of the sources of inputs, model results, any complication of model results—as in a spreadsheet, and the source for interpretation of the results.

All model results must be within parameters set by the numerical model developers (i.e., within mass balance targets) to be accepted.

As an alternative to direct simulation the use of statistical models will be explored in this project. Because a generic applicability is sought in the first phase of the work, statistical models (Jobson, 1996, Kilpatrick and Taylor, 1986, and Holley and Jirka, 1986) will be explored for their usefulness in this work. These provide an approach based on data analysis from around the U.S., although each might use a differing underlying data set. The assessment of these approaches can come from comparison against each other's results, other analytical models of transport and expert judgement.

Model Uncertainty

Since most of the model inputs are anticipated to have variability or uncertainty associated with them, the model is not expected to produce one single-valued result. Typically, only ranges or probability distributions of model outputs are justified from environmental simulation models. As such a set of appropriate scenarios will be constructed to illustrate the appropriate uncertainties in the model results. Characteristics of the problem and the model results will point to the appropriate scenarios. It is anticipated, however, that high, medium and low flow situations will be of interest. Others will be defined as appropriate.

Uncertainty analysis techniques that utilize all plausible combinations of input parameters will be used to test the Jobson empirical modeling results (Weaver et al., 2002, Weaver, 2004, Tillman and Weaver, 2006). This method will be modified from the software developed by Tillman and Weaver (2006) and adapted to the Jobson empirical calculations.

Document Retention

Model inputs and results that will form the basis of outputs from this project will be adequately documented for future tracing. The names and an outline of the contents of the files will be recorded in the lab notebooks of the participants. See Section A9 for more detail.

A8 Special Training/Certification

No special training is anticipated at the time of this writing.

A9 Documents and Records

All project documents will be stored in electronic form on Agency computers. The local “MyDocuments” synchronization feature will be used for storage and backup. The documents will be divided into two broad categories: records and non-records. “Records” will be used for all work produced by this project. “Non-records” will be used for information copies of documents.

The project is expected to produce, non-records that consist of informational copies of journal papers, agency reports and others. The records produced for the project will consist of data used in simulations, reduced data used in simulation and methods of data reduction, definition of model scenarios, model input files, model output files, interim reports (milestones) and a final report.

The project plan will be saved as a record under the directory and title:

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/Records/001ProjectPlan/

The QAPP will be saved as a record under the directory and title:

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/Records/002QAPP/Weaver-QAPP-surface water scenario modeling-revXX.docx

The “XX” will reflect the version number of the QAPP, beginning with “00” The version number is anticipated only to change if approved changes and additions are made to the initially-approved QAPP.

Each project participant will be supplied with the copy of the QAPP. Additionally the QAPP will be continuously available from the ORD O: drive. Each EPA participant will establish a similar directory structure for storage of their documents. They shall replace the Directory

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver

with a similar directory containing their name.

Data for this project are planned to be obtained from journal papers, published reports and other appropriate sources. These will be considered to be non-records. Electronic copies will be stored as described above. For example:

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/005NonRecords/Agency Reports

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/005NonRecords/ConsultantReports

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/005NonRecords/Literature

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/005NonRecords/OutsideCommunications

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/005NonRecords/StateData

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/005NonRecords/University

General documentation developed for publication will be saved in

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/050-Documentation

Model inputs are not considered fundamental data sources, but are to be documented with any associated model outputs. Electronic files shall be named so that the model used, date and characteristics of the input can be briefly identified in appropriately designed directories, AND associated with the corresponding model outputs. For example for the model "100"

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/Records/100-Modeling/aaa-ModelName

Where aaa is an arbitrary sequence number.

Supporting information for the model runs will be saved under appropriate directory titles, for example for the Jobson model:

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/Records/100-Modeling/001-Jobson

For the Jobson empirical model, and

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/Records/100-Modeling/001-Jobson/001-ReedAndStuckey

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/Records/100-Modeling/001-Jobson/002-SusquehannaTimeOfTravel

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/Records/100-Modeling/001-Jobson/003-Susquehanna Flow

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/Records/100-Modeling/001-Jobson/004-RiverMileData for Tioga-Chemung-Susquehanna

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/Records/100-Modeling/001-Jobson/005-RiverTracerData

Model inputs and outputs will also be documented in a laboratory notebook, giving the sense of the simulations performed and the locations of electronic computer files in the directories as indicated above. Models and versions used will be documented in the laboratory notebook.

For the separate scenarios that will be developed in this project they will be numbered and catalogued in the lab notebook. For example

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/Records/100-Modeling/001-Jobson/Scenario1

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/Records/100-Modeling/001-Jobson/Scenario2

Overall the electronic data scheme will follow:

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/ 001-ProjectPlan

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/ 002-QAPP

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/005NonRecords

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/005NonRecords/Literature

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/005NonRecords/AgencyReports

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/005NonRecords/

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/ 100-Modeling

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/ 100-Modeling/aaa-ModelName/Scenario1

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/ 100-Modeling /aaa-ModelName/Scenario2

Subdirectories from these major directories will be created as needed.

Model source code shall be stored in directories as follows:

MyDocuments/Research/workspace/RiverModel/src/riverModel

Java Class files shall be stored in

MyDocuments/Research/workspace/RiverModel/bin/riverModel

Results from test problems shall be stored as follows:

MyDocuments/Research/workspace/RiverModel/results

This directory structure follows the requirements of the Eclipse development environment (see section B10) used for this project.

Contractor (Shaw Environmental) Directory Structure

To match project 5b and other requirements, Shaw Environmental will follow a different directory structure:

C:\Projects\HydraFrac\

Then because of the multiple sites around the US it is more specific

C:\Projects\HydraFrac\PA_SRB\

And finally your TD Data path is

C:\Projects\HydraFrac\PA_SRB\RiverMile

Then the backup goes to the Kerr Facility IT archive drive path of

L:\Lab\CSMOS\8CS - Shaw Option 3 TD - 2011\8HF - HydraFrac
Then to the specific TD(s)

L:\Lab\CSMOS\8CS - Shaw Option 3 TD - 2011\8HF - HydraFrac\8HF116HF

Data files received from Shaw (by EPA) will be saved according to the structure described in the beginning of section A9.

Because this project is assigned a level 1 QA Category, all paper project records require permanent retention per Agency Records Schedule 501, *Applied and Directed Scientific Research.* Records will be stored in room 211 (Weaver's office) in the GWERD until they are transferred to GWERD's Records Storage Room. At some point in the future, paper records will be transferred to a National Archive facility.

All documentation shall provide enough detail to allow for reconstruction of the project activities. Documentation practices shall adhere to ORD PPM 13.2, "Paper Laboratory Records."

Records will be moved to the HF project O: drive when work is completed.

B1-B6, B8 Sampling and Measurement Requirements

The following list of sampling and measurement requirements appears in "EPA Requirements for Quality Assurance Project Plans " (EPA QA/R-5, EPA/240/B-01/003). These items were considered for this plan but were judged non-applicable to a literature, data evaluation, and modeling study.

B1 Sampling Process Design

B2 Sampling Methods

B3 Sample Handling and Custody

B4 Analytical Methods

B5 Quality Control

B6 Instrument/Equipment Testing, Inspection, and MaintenanceB8 Inspection/Acceptance of Supplies and Consumables

B7 Sampling and Measurement Requirements

B7 Instrument/Equipment Cailbration and Frequency

Calibration. The Jobson (1996) empirical approach is uncalibrated. Because the underlying dataset used to develop the approach used rivers of all sizes in the US (including the Mississippi) the empirical model applies anywhere in the US. A special study determined that the methods applied to Pennsylvania (Reed and Stuckey, 2002), with some exceptions, which will be used in this project.

For use of the empirical model the appropriate testing procedure is to demonstrate that the uncalibrated model results match data from a tracer experiment. Seven experiments that cover a range of flow conditions are being considered for testing the empirical model (Antietam Creek, Monocacy River, Tangipohoa River, Red River, Wind River, Mississippi River and the Yellowstone River). The last of these (Yellowstone River) was not used in generating the empirical equations—so it provides a test of the predictive capability of the method. Application to the other rivers is essentially equivalent to calibrating a numerical model, as the model is forced to match the experimental data. Calibrated models can only be said to represent the data to which they were calibrated—no extrapolation is demonstrated by calibration. The Yellowstone River application, in contrast, is an extrapolation of the method beyond its calibration data set. Thus model results which demonstrate correct simulation of the Yellowstone experiment would demonstrate a higher level of model testing than analogous calibration of a numerical model.

Goodness-of-fit for the empirical model will generally be taken by visual observation of concentration histories (breakthrough curves) at sampling locations, through professional judgment.

For models that require calibration testing, data are available from numerous USGS tracer experiments (Nordin and Sabol, 1974). In these cases, goodness-of-fit will be determined from quantitative measures (i.e, least squares). To support use of the empirical model, numerical models will be fitted to the same tracer data sets.

B9 Non-direct Measurements

The data needed for this project all fall under the category of non-direct measurements. These are discussed in items “A7 Quality Objectives and Criteria” and “D1 Data Review, Verification, and Validation”.

The data anticipated include:

- data on flows in specific rivers of interest that are available from USGS gages
- data on watershed characteristics
- USGS tracer study data
- data on discharges from publicly-owned and commercial waste water treatments that treat HF wastes
- data on concentration of typical flowback and produced water (FB/PW)
- data on concentrations of disinfection byproduct producing chemicals that created potential impacts on drinking water resources
- data on background concentrations of all chemicals of concern

Data Sources:

Four major data sources will be used for the project:

1) USGS data on flows and watershed characteristics are presented in a finalized, reviewed form on their web site (http://waterdata.usgs.gov/nwis/sw). These will be taken for selected river courses of interest and the following information will be gathered: average annual discharge, monthly average discharge, drainage area, location (latitude-longitude), gage elevation.
2) USGS tracer data, published in USGS reports will be accepted as being of acceptable quality. An early compilation (Nordin and Sabol, 1974) was used by Jobson (1996) as one part of the data for developing his regression equations. Other studies conducted since 1996 have potential usefulness for independent testing of the equations. One such experiment was conducted by McCarthy (2009) in the Yellowstone River.
3) Data submitted to state agencies or US EPA in fulfillment of legal requirements (i.e., national pollutant discharge elimination system (NPDES) required monthly monitoring; Pennsylvania mandated reporting of quantities of oil and gas waste). Data are available for Pennsylvania on treatment of oil and gas wastewaters and their disposal methods and locations. These shall be collected by Shaw Environmental according to the procedures and QAPP developed for HF project 5b on water acquisition.
4) Data on flowback and produced water for the Marcellus Shale will be used to estimate concentrations in wastewater, as the Pennsylvania data contains only waste volumes. For example, Rowan et al., 2011 compiled data on the Northern Appalachian basin of the US. These data are directly applicable to generating input conditions for this modeling. Some of the needed data include: disinfection byproduct-generation (i.e., Krasner et al., 2006) and

background concentration data for bromide, total dissolved solids and naturally occurring radioactive materials.

Data from the four above-mentioned sources will be accepted as being of sufficient quality for this project: USGS data streamflow data, data from USGS reports, data reported to state agencies for compliance, and peer-reviewed, published literature.

B10 Data Management and Hardware/Software Configuration

Data for this project will be stored as described in section "A9 Documents and Records," which includes electronic input and output files, spreadsheets and laboratory notebooks.

The PI is responsible for maintaining data files, including their security and integrity. All files will be stored (electronic) and labeled to identify this project.

Laboratory notebooks of the researchers will be the primary key to all data used in the project. The PI's (Weaver) notebook will summarize all data, models and model applications for the project. A spreadsheet/word document will be developed to summarize all available data. This spreadsheet will contain a description of the item, source, and location of computer files containing more information (if applicable). This spreadsheet will be continuously available to all project members by using the ORD O: drive. Ultimately the spreadsheet will become part of the project report.

The data management spreadsheet will be stored in

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/100-Modeling/aaa-ModelName/000-DataSummary

And will be named

SurfaceWaterScenarioDataManagement.xlsx

Similarly model runs will be catalogued in a spreadsheet/word document

The data management spreadsheet will be stored in

MyDocuments/Research/HF/SurfaceWaterScenario/Weaver/Records/Modeling

And will be named

SurfaceWaterScenarioModelRunManagement.xlsx

Data in hard copy form will be manually entered into Excel spreadsheets or model input files on designated GWERD staff computer and will given to the PI.

A minimum of ten percent of electronic data in spreadsheets or in model input files will be spot-checked to ensure accuracy of the transfer. If errors are detected during the spot-check, the entries will be corrected. Detection of an error will prompt a more extensive inspection of the data, which could lead to a 100% check of the data set being entered at that time if multiple errors are found. The checks shall be documented in lab notebooks to demonstrate that appropriate checking has been performed, and that corrections have been made. Spreadsheet cells that are corrected shall be colored to show where changes were made.

Model inputs and model outputs will be validated by initial and final reviews: This will include checking to assure that the model input files contain the intended input values, and after completing model runs, that model outputs correspond to the correct sets of inputs. When compiled for presentation, compilations (likely to be in spreadsheets) will be checked against actual output files, using the 10%/100% checking criteria described above.

USGS stream gage data will be used to generate parameter estimates needed for use in the Jobson equations. Treatment of these data shall be as follows:

Discharges and drainage areas will be obtained from the database developed under project 5b and its QA procedures.

Distances along rivers: Distances along rivers are calculated in ESRI software using built-in procedures. The calculated distances will be spot checked (minimum of 10%; 100% check if multiple errors found) using appropriate techniques (i.e., subdividing the river into segments, then adding the segments to assure that the results from both approaches are consistent). Checks will be documented in lab notebooks.

Slopes: Slopes are calculated from gage elevations and distances along the rivers. A hand check of calculated river slopes will be performed, using the criteria for data checking (minimum of 10%; 100% check if multiple errors found).

Hardware and Software Configuration

Hardware: Calculations will be performed with agency standard CTS and ORD computers. Two immediately available machines are in the possession of the PI: CTS Dell #CTS008316 and ORD Dell Latitude D630, decal #002507.

Software: Both of these machines use Windows XP. Standard software will be used in this project: Microsoft Office Word and Microsoft Office Excel are planned for data evaluation and generic screening calculations. Modeling codes such as WASP, QUAL2K, or others will be employed for the watershed simulations.

Java program development shall be undertaken using the Java Version 1.6 or higher and the Eclipse Development Environment. Eclipse is documented at http://www.eclipse.org/.

C1 Assessments and Response Actions

Model Performance Testing

The performance of all models used in this task will be tested against available USGS tracer data. These data will be used for ground truthing the model application as they will be used to answer the question of how well does the model represent actual conditions in the field. These assessments will be documented and reported as part of the project results.

USGS tracer data are available for numerous rivers, streams and creeks around the US (e.g., Nordin and Sabol, 1974, P.M. McCarthy, 2009). These experiments generally consist of release of a known mass of tracer dye into a flowing river. Concentration-versus- time data are collected at a number of downstream locations. These tracer data provide the means of testing numerical models, because the data directly incorporate travel time and turbulent dispersion of the tracer. The empirical calculations of Jobson (1996) permit calculation of travel time and concentration without calibration. Thus a test of this calculation method is its ability to replicate tracer experiment data. Several data sets will be selected from USGS tracer literature and used to test Jobson empirical results. Results from these tests will be documented in laboratory notebooks. Since numerous tracer experiments exist a set of data from Nordin and Sabol, 1974 will be used for the testing. Rivers/creeks will be chosen to cover the entire range of flow rates in the Nordin and Sabol data set. One or more data sets will be selected that were not used in development of the Jobson equations (Yellowstone River, McCarthy, 2009)Since models are inherently dependent on the choices made for their inputs, the response of the model to variation in inputs will be determined. Sensitivity analysis seeks to determine the response of the model to a unit change in each of its inputs. The results of sensitivity analysis allow an importance ranking of the parameters to be established, with the implication that the most important parameters should receive the most attention—i.e., additional data collection and refinement of estimated values.

Uncertainty analysis brings to the assessment, the combined influence of sensitivity to input parameters and the range of values seen in model application. In the planned work the parameters to be varied are:

Discharge concentration, flow rate, duration,

River flow: high, medium or low,

River characteristics: slope, drainage area, average annual discharge

Distance to nearest receptor.

Results from repeated simulation will determine if a consistent pattern of parameter importance exists. If so, this will be documented as a result of the simulations.

QA Audits

A Technical systems audit (TSA) will be done early enough in the project to allow for identification and correction of any issues that may affect data quality. It is anticipated it will be done after the QAPP is revised to incorporate the watershed simulations. It will be performed on a schedule determined by the GWERD QA Manager in cooperation with the PI. Detailed checklists, based on the procedures and requirements specified in this QAPP, related SOPs, and EPA Policies will be prepared and used during the audit. A QA assessment (comparable to an Audit of Data Quality on measurement projects) will be conducted on a representative sample of data. This assessment and its timing will be discussed during the TSA. These audits will be conducted with contract support from Neptune and Co., with oversight by Steve Vandegrift, QAM.

See Section C2 for how and to whom assessment results are reported.

Assessors do not have stop work authority; however, they can advise the PI if a stop work order is needed in situations where data quality may be significantly impacted, or for safety reasons. The PI makes the final determination as to whether or not to issue a stop work order.

For assessments that identify deficiencies requiring corrective action, the audited party must provide a written response to each Finding and Observation to the QA Manager, which shall include a plan for corrective action and a schedule. The PI is responsible for ensuring that audit findings are resolved. The QA Manager will review the written response to determine their appropriateness. If the audited party is other than the PI, then the PI shall also review and concur with the corrective actions. The QA Manager will track implementation and completion of corrective actions. After all corrective actions have been implemented and confirmed to be completed; the QA Manager shall send documentation to the PI and his supervisor that the audit is closed. Audit reports and responses shall be maintained by the PI in the project file and the QA Manager in the QA files, including QLOG.

At the conclusion of a TSA, a debriefing shall be held between the auditor and the PI or audited party to discuss the assessment results. Assessment results will be documented in reports to the PI, the PIs first-line manager, and the Technical Research Lead. If any serious problems are identified that require immediate action, the QAM will verbally convey these problems at the time of the audit to the PI.

The PI is responsible for responding to the reports as well ensuring that corrective actions are implemented in a timely manner to ensure that quality impacts to project results are minimal.

C2 Reports to Management

Progress reports will be made at the monthly project conference calls. These will include information on quality assurance and documentation.

All final audit reports shall be sent to the first-line manager of the PI, the Technical Research Lead, and copied to the PI. Audit reports will be prepared by the QA Manager with input from the QA support contractor where audit performance was delegated. Specific actions will be identified in the reports.

D1 Data Review, Verification, and Validation

Data review, verification, and validation will focus initially on the acceptability of literature data for simulation purposes. This review will rely on expert judgment, criteria presented in Section B9, and a broad knowledge of the literature on several topics including generalized transport in rivers, disinfection byproduct research and chemical transport.

In the generic modeling phase of the project, since specific rivers are not being simulated, calibration of models to field data will not be anticipated. If data arise that would allow a direct comparison, then these will be used to test the generic river approach.

Data or model results will not be released outside of the Robert S. Kerr Environmental Research Center until they have been reviewed, verified and validated as described below. The PI is responsible for deciding when project data can be shared with interested stakeholders in conjunction with the GWERDs Director's approval.

D2 Verification and Validation Methods

Quantitiative comparisons will be used when allowed by data availability. These will be used to develop a metric, say least squares, that can provide an objective fitting parameter. These are expected to allow for the actual river data to be shown to be within boundaries predicted by the scenario model results.

D3 Reconciliation with User Requirements

The project leader is likely to be a part of the writing team for the 2012 report to congress. Through this and the leadership of the theme lead (Stephen Kraemer), the model results will remain focused on the appropriate objectives. Dr. Kraemer will serve as a reviewer at each critical stage of the project.

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REVISION HISTORY:

Revision Number	Date Approved	Revision
0	9/10/11	New document
1	2/22/12	• A3, A4, Organization Chart: additional project personnel added • A6, Model Selection: additional text included on Jobson's technique • A6, Definition and Testing of a Simplified Scenario: text added on scenario development explanation of departure from original plan on generic simulations • Added description of Jobson (1996) equations • Updated timing of milestones on p. 10 • A7, deleted second paragraph in "Data with Known Quality" • A7, added section on "Documenting Code Development" • A7, added second paragraph to "Model Uncertainty" • A9, provided more detail on file structure for storing electronic copies and file naming convention • Added detail for Shaw Environmental data file structure • B7, added description of calibration and goodness-of-fit • B9,added detailed description of data that will be used and is considered acceptable

		• B10, added description of checks for each data type • C1, “Model Performance Testing,” added discussion on the use of tracer data to test Jobson empirical results • C1 subsurface example switched to surface water example • C1, “QA Aduits,” provided clarification on ADQs • References, additional references added